

Realization of the π -state in junctions formed by multi-band superconductors with a spin-density-wave.

A. Moor, A. F. Volkov, and K. B. Efetov

*Theoretische Physik III,
Ruhr-Universität Bochum, D-44780 Bochum, Germany*

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Using a simple model for Fe-based pnictides, we calculate the Josephson current I_J in a tunnel junction composed by such superconductors. We employ the tunnel Hamiltonian method and quasiclassical Green's functions. We study both the case of coexistence of the superconducting (Δ) and magnetic (SDW—spin density wave) order parameters and the case when only the superconducting order parameter exists. We analyze ideal and nonideal nesting and show that the current I_J depends on the mutual orientation of magnetization of the SDW only in the case of nonideal nesting.

It is found that the realization of the π -junction is possible in both cases. We show also that in $S_{++}/I/S_{+-}$ tunnel junctions an anomalous term $\sim I_{an} \cos \varphi$ may arise in the Josephson current and this result remains valid in the absence of the SDW (S_{++} and S_{+-} are superconductors with (Δ, Δ) respectively $(\Delta, -\Delta)$ order parameters in different bands and I denotes an insulating layer).

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Introduction. The superconducting order parameter (OP) in the BCS model Δ is either constant or angle-dependent as it occurs in anisotropic superconductors¹. Superconductors of new types discovered in last decades are characterized by a more complicated OP. For example, it is proposed that the OP in superconductors with heavy fermions may have the OP corresponding to the triplet pairing and having a vector structure². The OP in high- T_c superconductors depends on angles and in some of them corresponds to the singlet, so-called d -wave pairing: $\Delta(\alpha) = \Delta_0(\cos(k_x a_x) - \cos(k_y a_y))$, where $k_x = k_F \cos \alpha$, $k_y = k_F \sin \alpha$ are the components of the Fermi momentum k_F in the CuO layers³. This means that the OP turns to zero in certain directions and therefore nodes arise in the excitation spectra.

The OP in the recently discovered superconducting materials—Fe-based pnictides, which have rather high T_c ($\sim 60\text{K}$)⁴—is also nontrivial. These materials belong to a class of multi-band superconductors; their band structure consists of electron and hole bands. The OP in these bands may have not only different amplitudes but also opposite signs. If the OP in the hole and electron bands have different signs, one speaks of the s_{+-} -pairing—in contrast to the s_{++} -pairing in case of the same signs of the OP in different bands (see, for example, reviews 5–11). Investigating the structure of the OP in different types of superconductors is a very important task since this study may shed light on the mechanism of superconductivity in these materials.

One of the effective methods to determine the structure of the OP is the measurement of the Josephson current. For example, the sign change of the OP in high- T_c superconductors has been proven in experiments in which the critical Josephson current I_c was measured in a setup containing two Josephson junctions connected by a superconducting loop (i.e., on SQUID)³. The dc Josephson effect in multi-band superconductors has been studied theoreti-

cally in many papers^{12–19}. The calculations in Refs. 13 and 14 are focused on the multi-band superconductor MgB_2 , whereas the main attention of the authors of Refs. 15–19 is paid to the Fe-based pnictides. Agterberg et al.¹³ have shown that the Josephson $S/I/S_{mb}$ junctions may have a negative critical current I_c if the OP Δ is negative in some of the bands (here, S and S_{mb} mean single-band and multi-band superconductors, respectively, I stands for an insulating layer). This idea allows a simple physical interpretation. The Josephson current I_c in an $S/I/S_{mb}$ junction can be written as $I_c \propto \sum_{\alpha} \Delta_{\alpha} / R_{\alpha}$, where R_{α} is the resistance for electron transitions from the S superconductor to the band α in the S_{mb} superconductor. It is clear that if Δ_{α} is negative, for instance in the band with $\alpha = 1$, the current I_c may be also negative. This happens provided the resistance R_1 is sufficiently small. The ground state of the Josephson junction with negative I_c is called the π -state.

Note that the existence of the π -state of the Josephson junction is interesting in itself because such junctions can be used in practical applications (see, e.g., Ref. 20 and references therein). The π -state is realized in $S/F/S$ Josephson junctions and is being studied very actively (for reviews see Refs. 21–25). Therefore, there is a need both from the point of view of fundamental research and of the future applications to study the possible realizations of the π -state in Fe-based pnictides. In all publications mentioned above the presence of the spin density wave (SDW) in these materials is ignored. On the other hand, it is known that there is a region on the T - x -plane (temperature and doping level) where the superconducting and magnetic (SDW) phases co-exist.

In the present paper we calculate the Josephson current I_c in tunnel junctions formed by multi-band superconductors, i.e., in the $S_{mb}/I/S_{mb}$ junctions, both with an SDW and in the absence of the SDW. We show that the critical current I_c in junctions with the SDW consists of two terms. The first one is proportional to $\Delta_1 \Delta_r$ and does not depend

on the angle between the magnetization vectors $\mathbf{m}_{l,r}$ in the SDW on the left (l) and on the right (r). The second term is proportional to $\Delta_l \Delta_r (\mathbf{m}_l \cdot \mathbf{m}_r)$. This means that this component can be negative and, as we will show, it can prevail so that $I_c \propto \cos(2\theta)$, where 2θ is the angle between the vectors \mathbf{m}_l and \mathbf{m}_r . Thus, I_c may be negative in such junctions. We show also, that an anomalous term $I_{an} \cos \varphi$ arises in $S_{++}/I/S_{+-}$ junctions in addition to the ordinary Josephson current $I_{an} \sin \varphi$.

System under consideration. Model. We consider a tunnel $S_{mb}/I/S_{mb}$ junction. Each superconductor on the left and on the right is described by the Hamiltonian $\mathcal{H}_{l,r}$ which contains the superconducting and magnetic energies taken in the mean field approximation^{26–29}. Transitions of electrons between superconductors is described by the tunneling Hamiltonian

$$\mathcal{H}_T = \sum_{\mathbf{p}, \alpha, \beta} \{ \mathcal{T}_{\alpha\beta} \hat{a}_{\alpha,r}^\dagger \hat{a}_{\beta,l} + \text{H.c.} \} = \sum_{\mathbf{p}} \{ \hat{C}_r^\dagger \hat{H}_T \hat{C}_l + \text{H.c.} \}, \quad (1)$$

where the matrix elements $\mathcal{T}_{\alpha\beta}$ describe the electron tunneling between the same bands if $\alpha = \beta$, $\mathcal{T}_{\alpha\alpha} \equiv \mathcal{T}_\alpha$, and between different bands if $\alpha \neq \beta$. In the latter case one has $\mathcal{T}_{\alpha\beta} = \mathcal{T}_{\beta\alpha}^*$ for the identical superconductors at the left and right. We assume that the matrix elements $\mathcal{T}_{\alpha\beta}$ do not depend on momentum \mathbf{p} . The band $\alpha = 1$ (resp. 2) is assumed to be the hole (resp. electron) band. The $\hat{C} \equiv \hat{C}_{ans}$ operators are related to the \hat{a}_α operators as follows: $\hat{C}_{ans} = A_{ns}$ for $\alpha = 1$ and $\hat{C}_{ans} = B_{ns}$ for $\alpha = 2$. In the hole band one has $\hat{A}_{1n\uparrow} = \hat{a}_{1\downarrow}^\dagger$ for $n = 1$ and $\hat{A}_{1n\uparrow} = \hat{a}_{1\uparrow}$ for $n = 2$. In the electron band the relations $\hat{B}_{2n\uparrow} = \hat{a}_{2\uparrow}$ for $n = 1$ and $\hat{B}_{2n\uparrow} = \hat{a}_{2\downarrow}^\dagger$ for $n = 2$ take place. One can see that the labels α , n and s are the band, Gor'kov-Nambu and spin indices, respectively.

The operator \hat{H}_T can be written in terms of the matrices $\hat{\rho}$, $\hat{\tau}$ and $\hat{\sigma}$ which operate in the band, Gor'kov-Nambu and spin spaces: $\hat{H}_T = \hat{\Gamma} \cdot \hat{\tau}_3$. Here, the matrix $\hat{\Gamma}$ is given by

$$\hat{\Gamma} = \frac{1}{2} [\mathcal{T}_+ \hat{X}_{300} + \mathcal{T}_- - i(\mathcal{V}' \hat{X}_{210} - \mathcal{V}'' \hat{X}_{220})], \quad (2)$$

where $\mathcal{T}_\pm = (\mathcal{T}_1 \pm \mathcal{T}_2)/2$ and $\mathcal{V} \equiv \mathcal{V}' + i\mathcal{V}'' = \mathcal{T}_{12}$. The matrices \hat{X}_{ans} are defined as $\hat{X}_{ans} = \hat{\rho}_\alpha \cdot \hat{\tau}_n \cdot \hat{\sigma}_s$. It is worth making an important note. As is known, in tunnel junctions composed by single band superconductors, the relation $\mathcal{T}(p, p') = \mathcal{T}^*(-p, -p')$ holds which is a consequence of the time reversal symmetry. Therefore, the matrix elements $\mathcal{T}_{1,2}$ that describe tunneling between identical bands are real if we assume that these matrix elements do not depend on momenta p and p' . However, the matrix element $\mathcal{V} \equiv \mathcal{T}_{12}$ describes tunneling between different bands. In this case, the initial and final states are different and the idea about time reversal symmetry is not applicable. Therefore, the matrix element \mathcal{V} , generally speaking, is complex.

One can obtain the Eilenberger-like equation for quasiclassical Green's functions in the, e.g., right electrode with the self-energy part $\hat{\Sigma}_{T,r}$ which is related to the tunneling Hamiltonian: $\hat{\Sigma}_{T,r} = \hat{\Gamma} \cdot \hat{g}_l \cdot \hat{\Gamma}^\dagger$ ³⁰. The matrix \hat{g}_l in the self-energy part $\hat{\Sigma}_{T,r}$ is the quasiclassical Green's function in the left electrode. It can be found from the Eilenberger equation neglecting the self-energy $\hat{\Sigma}_{T,r}$ since we assume small

tunneling probability (the method of quasiclassical Green's functions is described in reviews 33–37). In the case of ideal nesting, this matrix function is given in Ref. 30. If the nesting is not ideal, this function acquires a more complicated form.

Josephson current. From the generalized Eilenberger equation one obtains the rate of the charge variation with time, e.g., in the right electrode: $(\partial_t Q_r + \partial_{t'} Q_r)|_{t=t'} = I_T$, where $Q_r = eN_r(0) \int d\epsilon \text{Tr} \{ \hat{X}_{300} \hat{g}_r^K \}$ with the density of states at the Fermi level $N_r(0)$ and \hat{g}_r^K is the Keldysh component of the Green's function. In equilibrium, this function is equal to $\hat{g}_r^K = (\hat{g}_r^R - \hat{g}_r^A) \tanh(\epsilon\beta)$ with $\beta = (2T)^{-1}$. The tunneling current in equilibrium is the nondissipative Josephson current I_J . It is given by

$$I_J = c_1 (4\pi i T) \sum_{\omega} \text{Tr} \{ \hat{X}_{330} [\hat{\Gamma} \hat{g}_l(\omega) \hat{\Gamma}^\dagger, \hat{g}_r(\omega)] \}, \quad (3)$$

where $c_1 = \pi e N_l(0) N_r(0) / 16$ and $\hat{g}_{l,r}(\omega)$ are the Green's functions in the left (right) electrodes in the Matsubara representation.

Ideal Nesting. Using Eqs. (2–3) we calculate the Josephson current between superconductors like Fe-based pnictides separated by a tunnel barrier. We start with the simplest case when the SDW is absent. Then, the trace in Eq. (3) is not zero only for the condensate component which has the form (we assume $|\Delta_{\text{hole}}| = |\Delta_{\text{electron}}| \equiv \Delta$)

$$\hat{g}_{l,r}(\omega) = \frac{\Delta}{\mathcal{D}} \begin{cases} \hat{X}_{323} \cos(\varphi/2) \pm \hat{X}_{013} \sin(\varphi/2) & \text{for } s_{+-}\text{-pairing,} \\ \hat{X}_{023} \cos(\varphi/2) \pm \hat{X}_{313} \sin(\varphi/2) & \text{for } s_{++}\text{-pairing,} \end{cases} \quad (4)$$

where $\mathcal{D} = \sqrt{\omega^2 + \Delta^2}$ and φ is the phase difference between the left and the right superconductors. We calculate the current I_J for different junctions: a) $S_{++}/I/S_{++}$, b) $S_{+-}/I/S_{+-}$ and c) $S_{++}/I/S_{+-}$. In the symmetric cases of identical superconductors forming the junction we obtain the standard formula $I_J = I_c \sin \varphi$ with different critical current

$$I_c/I_0 = |\mathcal{T}|^{-2} \begin{cases} |\mathcal{T}_1|^2 + |\mathcal{T}_2|^2 + 2\Re(\mathcal{V}^2) & \text{for } S_{++}/I/S_{++}, \\ |\mathcal{T}_1|^2 + |\mathcal{T}_2|^2 - 2\Re(\mathcal{V}^2) & \text{for } S_{+-}/I/S_{+-}, \end{cases} \quad (5)$$

where $I_0 = (\pi \Delta / 2e R_n) \tanh(\Delta/2T)$, $|\mathcal{T}|^2 = |\mathcal{T}_1|^2 + |\mathcal{T}_2|^2 + |\mathcal{V}|^2$ and $R_n^{-1} = 4\pi e^2 N_l(0) N_r(0) (|\mathcal{T}_1|^2 + |\mathcal{T}_2|^2 + |\mathcal{V}|^2)$ is the resistance of the junction in the normal state. In the case of an asymmetrical $S_{++}/I/S_{+-}$ junction we obtain a quite different result

$$I_J/I_0 = |\mathcal{T}|^{-2} [(|\mathcal{T}_1|^2 - |\mathcal{T}_2|^2) \sin \varphi + \Im(\mathcal{V}^2) \cos \varphi]. \quad (6)$$

As follows from Eqs. (5) and (6), in case of real tunneling matrix elements $\mathcal{T}_{1,2}$ and \mathcal{V} the critical current may be negative in junctions $S_{+-}/I/S_{+-}$ and $S_{++}/I/S_{+-}$. In the first case, I_c is negative if the interband transitions dominate, i.e., $\mathcal{T}_{1,2} \ll \mathcal{V}$. In the $S_{++}/I/S_{+-}$ junction, I_c changes sign at $|\mathcal{T}_1|^2 < |\mathcal{T}_2|^2$. These results resemble those obtained in Refs. 13–19, where the Josephson current in junctions of the type $S/I/S_{mb}$ has been studied.

However, if the tunneling matrix elements are complex, the obtained results do not reduce to those established earlier^{13–19}. Especially interesting is the result for the critical

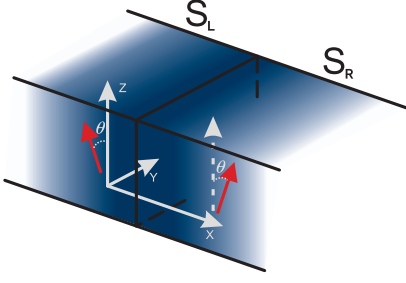


FIG. 1. (Color online.) Considered setup of the Josephson junction.

current in an $S_{++}/I/S_{+-}$ junction. In this case, the Josephson current has the form: $I_c \propto I_{c1} \sin(2\varphi) + I_{c2} \cos(2\varphi)$. This means that a spontaneous current arises even at zero phase difference; or a finite phase difference is established across the junction in a disconnected circuit. The presence of a spontaneous condensate current has been established earlier in different systems where the time-reversal symmetry breaking takes place. For example, this current arises in a superconducting loop containing a π -Josephson junction^{38,39} or in SF bilayer⁴⁰. The presence of the spontaneous current can be understood from the physical point of view as follows. Even if the global phase difference is zero ($2\varphi = 0$), the phase difference between the band with negative Δ and the band with positive Δ is not zero. Due to this, the interband transitions lead to the nonzero component current I_j . Note also, that there is a similarity of this effect and the anomalous proximity effect in S_{+-} system studied in Refs. 41 and 42.

Nonideal nesting. Now, we consider the most interesting case of the non-ideal nesting when the superconducting (Δ) and magnetic (SDW) order parameter may coexist in a certain interval of doping level x and temperature T ²⁶⁻²⁸, i.e., we introduce a parameter $\delta\mu_{\mathbf{p}}$, describing the mismatch of the effective Fermi surfaces of the bands. Then, the Green's function for the s_{+-} -pairing, in case $\varphi = 0$ and the magnetization vector oriented along the z -axis, has the form $\hat{g}_{+-} \equiv \hat{g}_{+-}(0, 0) = g_{030}\hat{X}_{030} + g_{100}\hat{X}_{100} + g_{123}\hat{X}_{123} + g_{213}\hat{X}_{213} + g_{300}\hat{X}_{300} + g_{323}\hat{X}_{323}$. For the s_{++} -pairing we have $\hat{g}_{++} \equiv \hat{g}_{++}(0, 0) = \tilde{g}_{023}\hat{X}_{023} + \tilde{g}_{030}\hat{X}_{030} + \tilde{g}_{123}\hat{X}_{123} + \tilde{g}_{130}\hat{X}_{130} + \tilde{g}_{213}\hat{X}_{213} + \tilde{g}_{300}\hat{X}_{300}$. That is, the matrices \hat{g}_{+-} and \hat{g}_{++} have a rather complicated form. In our notations for the S_{+-} system we follow previous papers^{29,30} and the quantities with tilde denote the according ones in the S_{++} system. However, only two terms— $g_{323}\hat{X}_{323}$, $g_{100}\hat{X}_{100}$ in \hat{g}_{+-} and $g_{023}\hat{X}_{023}$, $g_{130}\hat{X}_{130}$ in \hat{g}_{++} —contribute to the Josephson current.

If the phases $\varphi/2$ are different ($\pm\varphi/2$) and the angle $\theta \neq 0$ (see Fig. 1), the Green's functions in the left (right) superconductors $\hat{g}_{l,r}(\varphi, \theta)$ are expressed through the matrices $\hat{g}(0, 0)$ with the help of the unitary transformations: $\hat{g}_{l,r}(\varphi, \theta) = \hat{R}_{\pm\theta} \cdot \hat{S}_{\pm\varphi} \cdot \hat{g}(0, 0) \cdot \hat{R}_{\pm\theta}^\dagger \cdot \hat{S}_{\pm\varphi}^\dagger$, where the signs \pm relate to the left (right) electrodes. The transformation matrices are: $\hat{S}_{\pm\varphi} = \exp(\pm i\hat{X}_{330}\varphi/4)$ and $\hat{R}_{\pm\theta} = \exp(\pm i\hat{X}_{331}\theta/2)$. They can be called the rotation matrices in the Gor'kov-Nambu and spin spaces.

In the case of $S_{++}/I/S_{++}$ and $S_{+-}/I/S_{+-}$ junctions we obtain for the Josephson current

$$I_j/I_0 \propto \sin\varphi \cdot |\mathcal{T}|^{-2} \sum_{\omega} \{ \tilde{g}_{023}'^2 [|\mathcal{T}_1|^2 + |\mathcal{T}_2|^2 + 2\Re(\mathcal{V}^2)] + \tilde{g}_{130}'^2 \cos(2\theta) (\mathcal{T}_1\mathcal{T}_2 - |\mathcal{V}|^2) \} \quad (7)$$

and

$$I_j/I_0 \propto \sin\varphi \cdot |\mathcal{T}|^{-2} \sum_{\omega} \{ g_{323}'^2 [|\mathcal{T}_1|^2 + |\mathcal{T}_2|^2 - 2\Re(\mathcal{V}^2)] + g_{100}'^2 \cos(2\theta) (\mathcal{T}_1\mathcal{T}_2 - |\mathcal{V}|^2) \}, \quad (8)$$

respectively, where $\tilde{g}_{023}' = \tilde{\Delta}\zeta_+^{-1}|\psi|^{-2}\Im\{(\tilde{W}_{M0}^2 - \delta\tilde{\mu}_{\mathbf{p}}^2 + \zeta_+^2)\psi\}$, $\tilde{g}_{130}' = \omega_n\tilde{\Delta}\tilde{W}_{M0}\zeta_+^{-1}|\psi|^{-2}\Im\{\psi\}$, $g_{100}' = \Delta W_{M0}\zeta^{-1}|\chi|^{-2}\Im\{\chi\}$ and $g_{323}' = \Delta\zeta^{-1}|\chi|^{-2}(\zeta\Re\{\chi\} + \delta\mu_{\mathbf{p}}\Im\{\chi\})$, with $\psi = \sqrt{\tilde{W}_{M0}^2 + \tilde{\Delta}^2 + \omega_n^2 - \delta\tilde{\mu}_{\mathbf{p}}^2 - 2\zeta_+}$, $\zeta_+ = -i\sqrt{(\delta\tilde{\mu}_{\mathbf{p}}^2 - \tilde{W}_{M0}^2)\tilde{\Delta}^2 + \omega_n^2\delta\tilde{\mu}_{\mathbf{p}}^2}$, $\chi = \sqrt{W_{M0}^2 + (\zeta + i\delta\mu_{\mathbf{p}})^2}$ and $\zeta = \sqrt{\Delta^2 + \omega_n^2}$. We see that the angle-dependent part in Eqs. 7 and 8 differs from zero only if $\delta\mu_{\mathbf{p}} \neq 0$ (the condition of the non-ideal nesting).

In the case of the $S_{++}/I/S_{+-}$ junctions we obtain no angle dependent part

$$I_j/I_0 \propto |\mathcal{T}|^{-2} \sum_{\omega} \{ g_{013}'\tilde{g}_{023}' [|\mathcal{T}_1|^2 - |\mathcal{T}_2|^2] \sin\varphi + \Im(\mathcal{V}^2) \cos\varphi \}. \quad (9)$$

This formula looks like the corresponding expression for the case of an ideal nesting.

π -state. In principle, the realization of the π -state is possible in all three cases. The case c) of the $S_{++}/I/S_{+-}$ junction is discussed above. In the cases a) and b), i.e., in the $S_{++}/I/S_{++}$ and $S_{+-}/I/S_{+-}$ junctions it is possible to have the change of the sign of the critical current near T_c for sufficient large ratio of T_s/T_c .

However, the π -state is most easily realized and observed in the $S_{+-}/I/S_{+-}$ junction—at arbitrary temperature. To achieve that, one needs to adjust the tunneling probabilities related to the matrix elements $\mathcal{T}_{\alpha\beta}$ in a way as to make the first term in Eq. 8 (proportional to $g_{323}'^2$) vanish. Assuming the matrix elements \mathcal{T}_{α} real, this can be achieved, e.g., for the following ratios: $\mathcal{T}_2/\mathcal{T}_1 = 1$, $\Re\{\mathcal{T}_{12}\}/\mathcal{T}_1 = \sqrt{2}$, $\Im\{\mathcal{T}_{12}\}/\Re\{\mathcal{T}_{12}\} = 1/\sqrt{2}$. In this case, the critical current $I_c \propto \cos(2\theta)$ is proportional to cosine of the angle between the magnetization vectors in the leads. This, together with the mechanically favorable properties of the Fe-pnictides^{31,32}, makes the $S_{+-}/I/S_{+-}$ junction very attractive for possible applications in the quantum devices. In particular, the possibility of creating wires allows one to think of the realization of the so-called ϕ -junction (arbitrary phase shift, not only 0 or π) out of pieces of Fe-pnictide wire, put together mutually rotated and separated by an insulating layer—a chain of Josephson junctions.

Discussion. Starting from the generally accepted model for the Fe-based pnictides and a generic tunneling Hamiltonian, we investigated the Josephson current in the junctions consisting of two Fe-pnictides separated by an insulating layer: a) $S_{++}/I/S_{++}$, b) $S_{+-}/I/S_{+-}$ and c) $S_{++}/I/S_{+-}$,

where the indices indicate the pairing of the superconducting OP of the system. We find that, even in case of perfect nesting, the critical Josephson current shows unusual property for the $S_{++}/I/S_{+-}$ junction being finite for zero global phase difference (the so-called ϕ -junction). In case of perfect nesting, there also exists the possibility of a sign-change in the $S_{+-}/I/S_{+-}$ and $S_{++}/I/S_{+-}$ systems, thus enabling a π -state in the junction.

However, most easily the π -state is realized in the case of non-ideal nesting in the $S_{+-}/I/S_{+-}$ junction, where it is possible to achieve a cosine dependence of the critical Josephson current on the mutual orientation of the magnetiza-

tion vectors in the superconductors, $I_c \propto \cos(2\theta)$. Important ingredient for this effect is the co-existence of the SC and the SDW phases, as it occurs in the Fe-pnictides. It is not possible to achieve the pure cosine dependence of I_c on the mutual orientation of the magnetization vectors in the $S_{++}/I/S_{++}$ junction because the pre-factor of \tilde{g}_{023}^2 in Eq. 7 is always finite. In the $S_{++}/I/S_{+-}$ junction, there is no dependence on the mutual orientation of the magnetization vectors of the SDW.

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